

## METAL-AMMONIA COMPLEXES DISCLOSE A SECRET PERIODIC TABLE OF SOLVATED ELECTRON PRECURSORS

EVANGELOS MILIORDOS, *Chemistry and Biochemistry, Auburn University, Auburn, AL, 36849.*

Metal-ammonia complexes,  $[M(\text{NH}_3)_4]^{0,\pm}$ , are shown theoretically to have a  $M(\text{NH}_3)_4^{x+}$  positively charged core with one, two, or three outer electrons orbiting in its periphery. Our results reveal a new class of molecular entities (solvated electron precursors) which host outer electrons resembling atoms. The observed electronic shell model (1s, 1p, 1d, 2s, 1f, 2p, 2d) differs from that of the hydrogen-like model and resembles the jellium or nuclear shell model. This fact is attributed to the different effective electrostatic potential experienced by the outer electrons. Multi-reference and propagator approaches combined with diffuse basis sets are employed to calculate accurate geometries, ionization energies, electron affinities and vertical excitation energies. Our results are expected to trigger the interest of the experimental spectroscopy community.

